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TIME- AND PATH-ORDERED GREEN'S FUNCTIONS FOR NUCLEI

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Dedicated to Janusz Dąbrowski in honour of his 65th birthday

Time dependent Green's function methods provide a basic theory for nuclear dynamics and transport-properties such as related *e.g.* to heavy ion collisions. In the static limit this theory is also applicable to hot as well as zero-temperature nuclei. Retarded Green's functions are introduced in the non-equilibrium case while causal Green's functions have been used extensively for calculating ground-state properties of nuclei as have the very similar Brueckner methods. The purpose of this paper is to point out and clarify differences (and similarities) between these methods. In addition to some formal differences there are those resulting from accepted methods of application. Errors caused by using free Green's functions and related spectral-functions are pointed out. Only non-relativistic theories are discussed.

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1. Introduction

Many microscopic many-body calculations on properties of nuclei and nuclear matter have been made using causal (and anti-causal) Green's functions also referred to as chronological or time-ordered Green's functions. In addition there are many calculations done with Brueckner theory which are

in some respect (discussed below) very similar to these Green's functions techniques. Examples of recent works are those of Mahaux *et al.* [1, 2], Baldo *et al.* [3], Ramos *et al.* [4] and Köhler [5]. These methods are however strictly only applicable to ground state properties although some extensions to non-zero temperatures have been made [5, 6]. For finite-temperature and non-equilibrium studies these methods are however superseded by the path-ordered Green's functions techniques first introduced by Schwinger to study the Brownian motion of a quantum oscillator [7] and extended by Kadanoff and Baym [8] to the properties of many particle quantum systems in general. Subsequent work of Danielewicz [9, 10] as well as by Malfliet and coworkers [11, 12] use these techniques for nuclei. These works are for example of special interest for deriving mean fields *etc.* for transport-equations applicable to collisions between nuclei.

It appears important to establish a comparison between the non-equilibrium methods using retarded functions in the static zero-temperature limit and the previous works using causal Green's functions because there are many similarities but perhaps more interesting some formal differences. These differences have caused some confusion when results of calculations have been reported using the retarded Green's functions [13] for ground-state nuclear matter, which prompts this publication. Formal differences have already been pointed out in previous works *e.g.* [1, 10]. The purpose of this paper is to point out these differences more explicitly especially as regards the calculation of mean fields.

The properties of the various Green's functions and their relations are found in several references [8, 14, 15]. A summary of some relations *etc.* necessary for our discussion is given in Sec. 2. Definition of effective interactions and mean fields are given in Secs 3 and 4 for the causal (as well as Brueckner) and retarded case respectively. Differences between the results of applying these theories are pointed out in Sec. 5. Sec. 6 is a summary and a discussion follows in Sec. 7.

2. Green's functions

Let us consider an infinite nuclear medium. Although we shall later discuss this medium in equilibrium let us first consider the general case of non-equilibrium. It is then convenient to define Green's functions:

$$g^{<}(p) = -\frac{1}{i\hbar}a(p)F(p), \quad (1)$$

$$g^{>}(p) = \frac{1}{i\hbar}a(p)[1 - F(p)]. \quad (2)$$

Here $p = (\omega, \mathbf{p})$ and $a(p)$ is the spectral function while $F(p)$ is a distribution-function. These two Green's functions (correlation functions) completely

describe the one-particle properties of the system. In the case of equilibrium $F(p) \equiv f(\omega)$ one has in the usual notation

$$f(\omega) = \frac{1}{1 + e^{\beta(\omega - \mu)}}. \quad (3)$$

In this case one finds

$$g^>(p) = -e^{\beta(\omega - \mu)} g^<(p) \quad (4)$$

and only one function g is sufficient. The well-known Kadanoff–Baym equations describe the time-evolution of the functions $g^>$ and $g^<$. It is however at this point convenient to introduce the advanced and retarded functions. From the Kadanoff–Baym equations one finds (see *e.g.* Ref. [11])

$$g^{\pm}(p) = \frac{1}{\omega - p^2/2m - \Sigma^{\pm}(p) \pm i\epsilon}, \quad (5)$$

where $\Sigma^{\pm}(p)$ is the mean field to be defined later. One can introduce chronological and antichronological functions F^c and F^a by

$$F^c = F^{\pm} + F^<, \quad (6)$$

$$F^a = -F^{\pm} + F^>. \quad (7)$$

From the last two equations and Eq. (1) and Eq. (2) one finds a convenient expression for the spectral-function

$$a(p) = i\hbar \left(\frac{2i \operatorname{Im} \Sigma^{(+)}(p)}{[\omega - p^2/2m - \operatorname{Re} \Sigma^{(+)}(p)]^2 + [\operatorname{Im} \Sigma^{(+)}(p)]^2} \right). \quad (8)$$

In the limit of small absorption, $\operatorname{Im} \Sigma \ll 1$ one can consider using the quasi-particle approximation

$$a_{qp}(p, \omega) = 2\pi\hbar\delta(\omega - \epsilon_p)Z(p, \omega) \quad (9)$$

with the quasiparticle strength Z given by

$$Z(p) = \left(1 - \left(\frac{\partial \operatorname{Re} \Sigma^{+}(p, \omega)}{\partial \omega} \right)_{\omega=\epsilon_p} \right)^{-1} \quad (10)$$

and the energy ϵ_p defined by

$$\epsilon_p = \frac{p^2}{2m} + \operatorname{Re} \Sigma^{+}(p, \epsilon_p). \quad (11)$$

An even simpler approximation is obtained with $Z = 1$. This is referred to as the *quasi-classical* limit and for an infinite homogeneous medium in thermal equilibrium one finds the following *free* (or unperturbed) Green's functions

$$g_0^c(p) = \frac{1 - n(p)}{\omega - \epsilon_p + i\epsilon} + \frac{n(p)}{\omega - \epsilon_p - i\epsilon}, \quad (12)$$

$$g_0^a(p) = \frac{1 - n(p)}{\omega - \epsilon_p - i\epsilon} + \frac{n(p)}{\omega - \epsilon_p + i\epsilon}, \quad (13)$$

$$g_0^<(p) = 2\pi i n(p) \delta(\omega - \epsilon_p), \quad (14)$$

$$g_0^>(p) = 2\pi i (1 - n(p)) \delta(\omega - \epsilon_p), \quad (15)$$

with a mean field included so that ϵ_p is the single-particle energy including this mean field and $n(p)$ are occupation-numbers at thermal equilibrium defined by Eq. (3) with $\omega = \epsilon_p$ *i.e.*

$$n(p) = \frac{1}{\exp(\beta(\epsilon_p - \mu)) + 1}. \quad (16)$$

Perturbation schemes are developed in terms of these unperturbed functions.

As noted after Eq. (4) only one Green's function is necessary in the equilibrium situation. This is often chosen to be the causal (or chronological) function g^c as is the case in many ground state calculations. For example the mean field that is calculated is then the causal mean field Σ^c . For *non-equilibrium* systems two Green's-functions are however needed. In the equilibrium limit the mean field that one calculates is the advanced Σ^+ that for example is needed for calculating the spectral function defined by Eq. (8) and the propagator g^+ in Eq. (5). In thermal equilibrium an important relation between chronological and retarded functions exists (see *e.g.* Ref. [10]):

$$\text{Re } \Sigma^c(p) = \text{Re } \Sigma^\pm(p), \quad (17)$$

$$\text{Im } \Sigma^c(p) = \tanh(\tfrac{1}{2}\beta(\omega - \mu)) \text{Im } \Sigma^+(p). \quad (18)$$

At temperature $T = 0$ this becomes especially simple. There is in this case only a difference in sign between the imaginary parts of the chronological and retarded mean fields. As a consequence the spectral-function will in this case be the same if calculated by Eq. (8) with either Σ^c or Σ^+ . However for $T \neq 0$ this is no longer the case.

Although it may seem sufficient to show these general relations it seems necessary to investigate to what extent these are valid in the approximations used in actual calculations.

We find it illuminating to make this investigation in an approximation in which the mean fields are calculated to second order in the interaction V .

3. Chronological mean field

Using the chronological method one defines diagonal elements of the effective interaction by

$$\begin{aligned} \langle \mathbf{p}, \mathbf{p}' | T^c(\Omega) | \mathbf{p}, \mathbf{p}' \rangle &= \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}, \mathbf{p}' \rangle + \\ &+ \sum_{\mathbf{p}'', \mathbf{p}'''} \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}'', \mathbf{p}''' \rangle g^c(\mathbf{p}'') g^c(\mathbf{p}''') \langle \mathbf{p}'', \mathbf{p}''' | T^c(\Omega) | \mathbf{p}, \mathbf{p}' \rangle. \end{aligned} \quad (19)$$

(To simplify the expressions momentum and energy conservations are not explicit in this and the following equations.) The calculations are however done with free propagators g_0^c and in second order in the interaction V one then obtains after doing the ω'', ω''' integrations.

$$\begin{aligned} \langle \mathbf{p}, \mathbf{p}' | T_2^c(\Omega) | \mathbf{p}, \mathbf{p}' \rangle &= \sum_{\mathbf{p}'', \mathbf{p}'''} | \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}'', \mathbf{p}''' \rangle |^2 \\ &\times \left(\frac{(1 - n(\mathbf{p}''))(1 - n(\mathbf{p}'''))}{\Omega - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} - \frac{n(\mathbf{p}'')n(\mathbf{p}''')}{\Omega - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} - i\eta} \right). \end{aligned} \quad (20)$$

The mean field is given by

$$\Sigma^c(\mathbf{p}, \omega) = \sum_{\mathbf{p}', \omega'} \langle \mathbf{p}, \mathbf{p}' | T^c(\omega + \omega') | \mathbf{p}, \mathbf{p}' \rangle g^c(\mathbf{p}', \omega') \quad (21)$$

and in second order one gets with g^c substituted by g_0^c

$$\begin{aligned} \Sigma_2^c(\mathbf{p}, \omega) &= \sum_{\mathbf{p}', \mathbf{p}'', \mathbf{p}'''} | \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}'', \mathbf{p}''' \rangle |^2 \\ &\times \left(\frac{(1 - n(\mathbf{p}''))(1 - n(\mathbf{p}'''))n(\mathbf{p}')}{\omega + \epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} + \frac{n(\mathbf{p}'')n(\mathbf{p}''')(1 - n(\mathbf{p}'))}{\omega + \epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} - i\eta} \right). \end{aligned} \quad (22)$$

It is of interest to compare this with what one finds from Brueckner theory. The (diagonal element of the) Brueckner effective interaction K usually neglects the hole-hole ladders and is defined by

$$\begin{aligned} \langle \mathbf{p}, \mathbf{p}' | K(\Omega) | \mathbf{p}, \mathbf{p}' \rangle &= \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}, \mathbf{p}' \rangle + \sum_{\mathbf{p}'', \mathbf{p}'''} \langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}'', \mathbf{p}''' \rangle \\ &\times \frac{(1 - n(\mathbf{p}''))(1 - n(\mathbf{p}'''))}{\Omega - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} \langle \mathbf{p}'', \mathbf{p}''' | K(\Omega) | \mathbf{p}, \mathbf{p}' \rangle. \end{aligned} \quad (23)$$

We have *assumed* the same single particle spectrum ϵ_p although in Brueckner theory it is often defined differently as discussed in Sec. 7.

The Brueckner energy E^B is given by

$$E^B = \sum_p \frac{n(p)p^2}{2m} + \frac{1}{2} \sum_{p,p'} n(p)n(p') \langle p, p' | K(\epsilon_p + \epsilon_{p'}) | p, p' \rangle. \quad (24)$$

By the (Landau) definition of single particle energy one has [16]

$$\epsilon_p = \frac{dE^B}{dn(p)}.$$

With E^B calculated to second order in the interaction V one obtains a term exactly like Eq. (22) with $\omega = \epsilon_p$. The first term in Eq. (22) is obtained from the variation with respect to $n(p)$ and $n(p')$ while the second term comes from the variation with respect to $n(p'')$ and $n(p''')$. The second term is usually referred to as a Brueckner second order rearrangement energy.

4. Retarded mean field

The retarded effective interaction T^+ is defined by (see *e.g.* [9, 11])

$$\begin{aligned} \langle p, p' | T^+(\Omega) | p, p' \rangle &= \sum_{p'', p'''} \langle p, p' | V | p'', p''' \rangle \\ &+ \frac{g^>(p'')g^>(p''') - g^<(p'')g^<(p''')}{\Omega - \omega'' - \omega''' + i\eta} \langle p'', p''' | T^+(\Omega) | p, p' \rangle. \end{aligned} \quad (25)$$

The retarded effective interaction to be compared with Eq. (20) is given by

$$\begin{aligned} \langle p, p' | T_2^+(\Omega) | p, p' \rangle &= \sum_{p'', p'''} |\langle p, p' | V | p'', p''' \rangle|^2 \\ &\times \left(\frac{(1 - n(p''))(1 - n(p'''))}{\Omega - \epsilon_{p''} - \epsilon_{p'''} + i\eta} - \frac{n(p'')n(p''')}{\Omega - \epsilon_{p''} - \epsilon_{p'''} + i\eta} \right). \end{aligned} \quad (26)$$

One finds that the only difference from T^c lies in the sign of the last $i\eta$. The mean field Σ^+ is given by

$$\begin{aligned} \Sigma^+(p, \omega) &= -i\hbar \sum_{p', \omega'} [\langle p, p' | T^+(\omega + \omega') | p, p' \rangle g^<(p', \omega') \\ &+ \langle p, p' | T^<(\omega + \omega') | p, p' \rangle g^-(p', \omega')] \end{aligned} \quad (27)$$

with $T^<$ given by

$$\begin{aligned} \langle \mathbf{p}, \mathbf{p}' | T^<(\omega + \omega') | \mathbf{p}, \mathbf{p}' \rangle &= i\hbar \sum_{\mathbf{p}'', \mathbf{p}'''} \langle \mathbf{p}, \mathbf{p}' | T^+ | \mathbf{p}'', \mathbf{p}''' \rangle \\ &\times g^<(\mathbf{p}'', \omega'') g^<(\mathbf{p}''', \omega''') \langle \mathbf{p}'', \mathbf{p}''' | T^- | \mathbf{p}', \mathbf{p} \rangle \end{aligned} \quad (28)$$

and one finds in second order after substituting with free propagators

$$\begin{aligned} \Sigma_2^+(\mathbf{p}, \omega) &= \sum_{\mathbf{p}', \mathbf{p}'', \mathbf{p}'''} |\langle \mathbf{p}, \mathbf{p}' | V | \mathbf{p}'', \mathbf{p}''' \rangle|^2 \\ &\times \left(\frac{(1 - n(\mathbf{p}''))(1 - n(\mathbf{p}'''))n(\mathbf{p}')}{\omega + \epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} - \frac{n(\mathbf{p}')n(\mathbf{p}'')n(\mathbf{p}''')}{\omega + \epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} \right. \\ &\left. + \frac{n(\mathbf{p}'')n(\mathbf{p}''')}{\omega + \epsilon_{\mathbf{p}'} - \epsilon_{\mathbf{p}''} - \epsilon_{\mathbf{p}'''} + i\eta} \right), \end{aligned} \quad (29)$$

where the last term comes from the second term in Eq. (27).

5. Comparison between chronological and retarded potentials

Comparing Eq. (29) with Eq. (22) one finds that the real parts of Σ^c and Σ^+ are identical as required by the general result given by Eq. (17). At temperature $T = 0$ the imaginary parts due to the first terms of both Σ^c in Eq. (22) and Σ^+ in Eq. (29) are equal to zero below the Fermi-energy because of the Pauli-blocking. The same is true for the second term above the Fermi-energy. The difference then is in the imaginary parts of the second term which have opposite signs and this is in agreement with Eq. (18) and discussion below this equation.

For temperatures $T \neq 0$ the situation is not that simple. Both of the terms contribute both below and above the Fermi-energy as is obvious with $n(\mathbf{p})$ given by Eq. (16). One finds however that

$$\text{Im } \Sigma_2^+(\mathbf{p}, \omega) \propto \exp(\beta(\epsilon_{\mathbf{p}''} + \epsilon_{\mathbf{p}'''} - 2\mu)) + \exp(\beta(\epsilon_{\mathbf{p}'} - \mu)), \quad (30)$$

$$\text{Im } \Sigma_2^c(\mathbf{p}, \omega) \propto \exp(\beta(\epsilon_{\mathbf{p}''} + \epsilon_{\mathbf{p}'''} - 2\mu)) - \exp(\beta(\epsilon_{\mathbf{p}'} - \mu)). \quad (31)$$

But $\epsilon_{\mathbf{p}'} = \epsilon_{\mathbf{p}''} + \epsilon_{\mathbf{p}'''} - \omega$ because of energy-conservation in the imaginary parts. Therefore

$$\text{Im } \Sigma_2^+(\mathbf{p}, \omega) \propto \exp(\beta(\epsilon_{\mathbf{p}''} + \epsilon_{\mathbf{p}'''} - \mu))(e^{-\beta\mu} + e^{-\beta\omega}), \quad (32)$$

$$\text{Im } \Sigma_2^c(\mathbf{p}, \omega) \propto \exp(\beta(\epsilon_{\mathbf{p}''} + \epsilon_{\mathbf{p}'''} - \mu))(e^{-\beta\mu} - e^{-\beta\omega}). \quad (33)$$

It is then easy to verify that $\tanh(\frac{1}{2}\beta(\omega - \mu)) \text{Im } \Sigma_2^+(\mathbf{p}, \omega) = \text{Im } \Sigma_2^c(\mathbf{p}, \omega)$ which is in exact agreement with Eq. (18).

6. Summary

Most nuclear matter calculations using Green's function or the, in practice, very similar Brueckner method have been done using effective interactions and mean fields defined by chronological Green's functions [1-6]. Only a few have been done with retarded Green's functions [12, 13]. The retarded Green's function method is more general being well suited also for non-zero temperature as well as non-equilibrium situations. Differences between the two methods exist in the limit of zero temperature. It is important to investigate these. In this paper it is only investigated in a second order perturbation expansion with respect to the interaction V . This may seem a limitation but one may in fact also explore the differences in an expansion to second order of the effective interaction; defined by chronological or retarded Green's functions. The conclusions are the same [17]. The important differences in analytic structure are already seen in second order. It is, we think, simpler for the retarded (or advanced) functions which are analytic in either the upper or the lower half-plane while the chronological functions have a more complicated analytic structure leading to complicated integrations and are of course only applicable at zero temperature.

Some general relations between the mean fields are readily established and given by Eq. (17) and Eq. (18). These relations were also found to be satisfied by the approximate treatments above. But some caution has to be taken when applying these methods in order that the mean fields satisfy the Eqs (17) and (18). In Brueckner theory the second order rearrangement energy has to be included. In the chronological formulation we have already seen in Sec. 3 that this term is included if hole-hole ladders are included in the effective interaction. In the retarded mean field the second order term, i.e. the second term in Σ^+ defined by Eq. (27) has to be included. The importance of this term should therefore not be forgotten. It was apparently first recognized by Malfliet *et al.* [11]. It is in fact very different in its structure (and numerical value) compared to the second order Brueckner rearrangement energy [13]. At zero temperature one finds in fact that the two methods differ only in the sign of the imaginary part of this particular term. It is non-zero only for states below the fermi-surface.

It is important to realize that although the effective interaction in Brueckner theory by definition neglects intermediate hole-states as seen in Eq. (23) this theory is still very similar to the chronological Green's function method as it for example gives the same expression for Σ_2^c as shown above.

7. Discussion

The equality between the three methods at zero temperature, the Brueckner, the chronological and the path ordered Green's functions has been

demonstrated to second order in the interactions. There is only a trivial difference in signs of some imaginary parts. At higher orders there is a difference but the only real difference is between the Brueckner method and the Green's function methods because (usually) Brueckner theory does not include hole-hole propagators in the effective interaction. The two Green's function methods should give rather similar results. The effect of including hole-hole propagators has been investigated to some extent. It is relatively small at normal density. The effect on energies is typically a few MeV as already found in early calculations. This is confirmed by more recent calculations as seen for example in Ref. [18] especially Fig. 2. The effect on the calculation of spectral functions is shown in Ref. [13] and it is also minimal. It is of course important to realize that hole propagations as concerns the mean field is included in the Brueckner second order rearrangement energy *albeit* to a lower order than in the Green's functions methods. With present-day computing power there is however no real reason to ignore the hole-hole ladders. This leads to a more consistent application of the Green's functions method applied to non-equilibrium dynamics and heavy ion collisions. It may also be important for the high densities reached in these collisions with increased phase-space for hole propagations.

In our analysis we have assumed the single particle energies in the propagators to be the same in all three cases. In Brueckner theory there is however a common practice to neglect the second order rearrangement mean field in the propagators defining the effective interaction K *i.e.* in the energies ϵ_p in Eq. (23). (For an exception see Ref. [3]). In other words the Brueckner choice for single particle energies ϵ_p^B to be used in the calculation of the K -matrix equation Eq. (23) is given by

$$\epsilon_p^B = \frac{p^2}{2m} + \text{Re } \Sigma_1(\epsilon_p^B, p),$$

where Σ_1 is the first order mean field *excluding* the Brueckner second order rearrangement energy. There is good reason for this choice because in the diagrammatic analysis one finds the second order insertions to be "off the energy shell" and therefore they contribute little to the total energy. This was already pointed out by Brueckner and coworkers [16]. In contrast the Green's function methods use the full field Σ (including the second order Brueckner field) in the propagators. Because the Green's functions g are approximated by free field functions g_0 one obtains quasi-particle energies defined by Eq. (11). This implies that the ω integrations are expected to give an average value located at the quasi-particle peak. It is well known however that the spectral functions are heavily skewed (see *e.g.* Ref. [13]) and a lower average value such as given by the Brueckner choice ϵ_p^B seems more reasonable. This may lead to significant numerical differences between

Brueckner and Green's function calculations. The practice of using the free field functions g_0 when applying the Green's function methods is an untested approximation. It is our belief that a better approximation is called for.

This is also suggested by a related error committed when calculating the total energy from the sum rule

$$E = 2 \int_{-\infty}^{\mu} d\omega \int_{-\infty}^{+\infty} \frac{d^3 p}{(2\pi\hbar)^3} \left(\frac{p^2}{2m} - \omega \right) a(\mathbf{p}, \omega)$$

with the spectral-function given by a quasi-classical approximation

$$a(\mathbf{p}, \omega) = 2\pi\hbar\delta(\omega - \omega_0)$$

as in Ref. [18]. An improved approximation, the extended quasiparticle approximation (EQP) for the spectral-function was in Ref. [13] shown to lead to an important correction. It was in fact found that the second order rearrangement energy (the hole-hole term) should be excluded in this sum rule or in other words that this energy does not contribute to the average energy $\omega_h(\mathbf{p})$ of a hole. Also note that the Brueckner choice of single particle energy ϵ_p^B defined above, also equals this average energy experimentally referred to as the (negative of) removal energy of a nucleon.

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